

Comparison of the Xenocs 2D and 3D optics on a **mar- μ X** data collection system

Claudio Klein, Marresearch GmbH, Norderstedt

Application Note 20Jun08

Introduction

In this study, we have used a *mar_{px}* system consisting of a *mar345* image plate detector, a *mar_{diff}* goniometer system and a Genix Cu High Flux generator operated at 50kV/1mA (50 W) to compare the performance of two different types of optics:

- a) Xenocs Fox 2D Cu 10_30
- b) Xenocs Fox 3D Cu 14_39

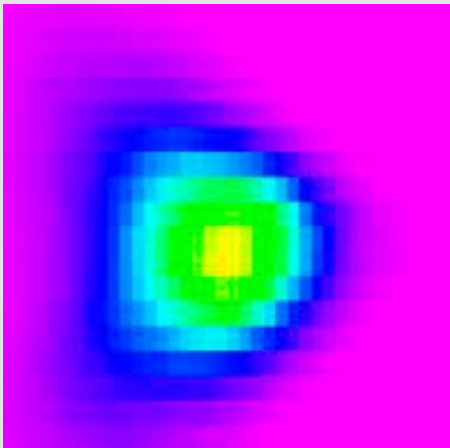
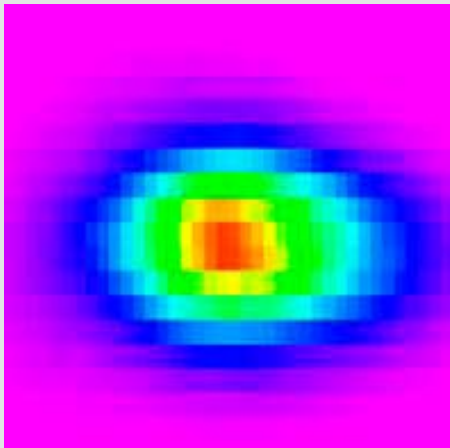
The Fox 3D CU 14_39 mirror features an optimized high precision ellipsoidal substrate and a state-of-the-art multilayer to achieve a beam with better focusing properties and higher flux density than the Fox 2D Cu 10_30 optics.

Two crystals were used in this study:

- 1.) a large lysozyme crystal (~350 μ m in all dimensions)
- 2.) a mid-size lysozyme crystal (~180 μ m)



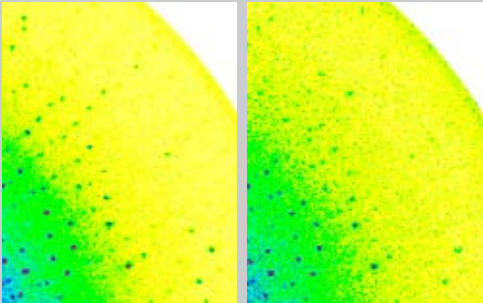
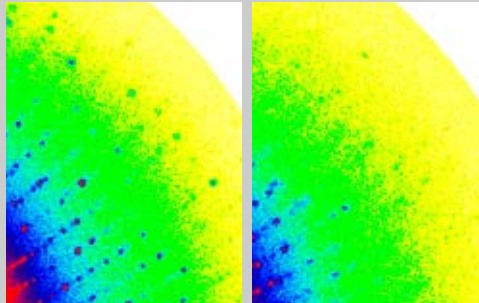


Technical Data of Optics

	FOX 2D Cu 10_30	FOX 3D Cu 14_39
Beam in focus		
The picture show an area of 0.5 x 0.5. The color coding reflects the measured intensity of the beam.		
Distance source - optic center	10 cm	14 cm
Distance optic center - focus	30 cm	39 cm
Spot size in focus	230 x 230 μ m ²	190 x 190 μ m ²
Typical flux	> 2 x 10 ⁸ photons/sec	> 3 x 10 ⁸ photons/sec
Divergence	4.8 x 4.8 mrad ²	5.4 x 5.4 mrad ²

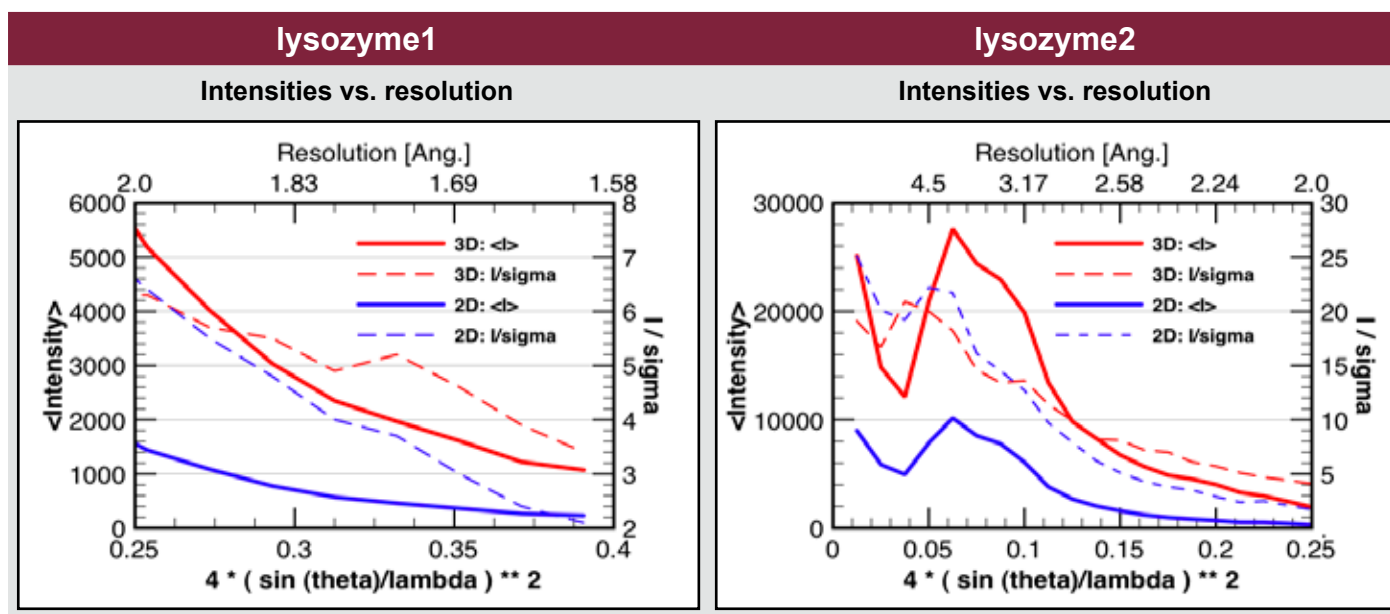
Data collection and processing

The data for all crystals were collected on the same GeniX generator and the same *mar₃₄₅ dtb* detector system. When exchanging the mirrors, the beam was carefully realigned. Data were processed using mosflm & scala. The data set of the lysozyme1 crystal collected with the 3D optics suffered from an unstable cryo-cooler (variations of temperature of 20 deg.). This explains the higher R-factors despite much stronger intensities.

		lysozyme1		lysozyme2	
Crystal					
Diffraction pattern	The pattern for the 3D optics is on the left hand side of each crystal type.				
Space group		P 4 ₃ 2 ₁ 2			
Unit cell axes		a=79.1 b=79.1 c=37.9 Ang.			
High resolution limit		1.60 Ang.		2.0 Ang.	
Mosaicity		0.3°		0.9°	
Size of crystal		450µm x 300µm x 250µm		150µm x 170µm x 200 µm	
Distance crystal-detector		100 mm		120 mm	
Exposure time per image		90 sec		300 sec	
Total no. of images		63		90	
Delta-φ per image		1.0°		1.0°	
Optics		3D	2D	3D	2D
Completeness	all / last shell	86.0 / 89.6 %	86.4 / 89.5 %	92.1 / 90.3	78.5 / 76.6
Multiplicity	all / last shell	5.3 / 5.1	5.3 / 5.1	6.4 / 5.5	5.7 / 5.4
Rsym	all / last shell	7.3 / 20.3 %	6.5 / 33.5	6.0 / 17.0	7.2 / 45.1
<Intensity>	all / last shell	9056 / 1071	2755 / 233	10134 / 1939	3298 / 300
I / σ	all / last shell	16.7 / 5.5	18.1 / 3.1	23.2 / 7.0	20.9 / 2.0

Data comparison

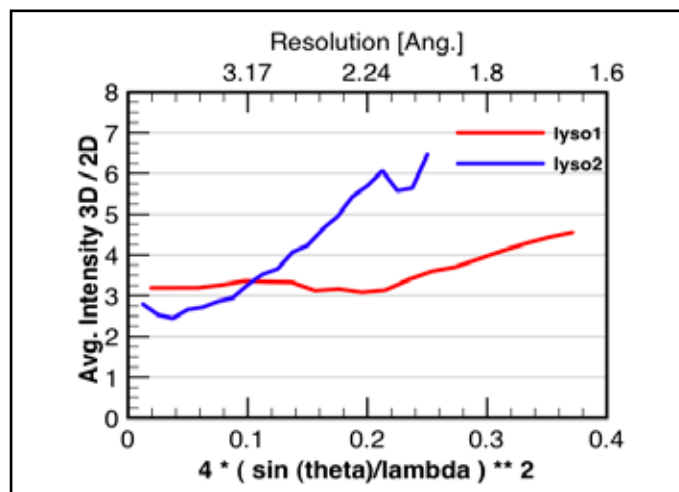
In the plots given below, the data collected with the 3D optic are drawn in red, the ones collected with the 2D optic are drawn in blue, respectively. The I/σ values (dotted lines) scale to the y-axis on the right hand side of the plot. For sake of clarity, for the well diffracting larger crystal only the high resolution ranges between 2.0 and 1.6 Ang. resolution are plotted.



For both the large crystal (lysozyme1) and the smaller crystal (lysozyme2) the 3D data show much larger net intensity values in all resolution shells than the 2D data. In particular at higher resolution, this also applies to I/σ -values. The difference of performance between the 3D and the 2D optic becomes more obvious when looking at the smaller crystal.

The picture on the right hand side shows the ratio of the average net intensity of the diffraction data from both optics. For the large crystal we see a constant ratio of approx. 3 times more intensity up to 2 Ang. resolution. For higher resolution shells, the factor increases to 4.5.

For the smaller crystal, the ratio is less linear, meaning that the smaller crystal benefits even more from the better beam quality of the 3D optic. In fact, a reasonable resolution limit for the chosen exposure time for the 2D optic was at about 2.2 Ang. while the data from the 3D optic extended to 1.9 Ang.



Conclusion

The data collected here suggest that at least a two-fold increase in observed diffracted intensity can be expected from the Fox3D Cu 14_39 optic as compared to the 2D optic. This increase translates in better I/σ -ratios and possibly higher resolution. For smaller crystals, the performance difference is expected to further increase.